

# Exact valence bond entanglement entropy and probability distribution in the XXX spin chain and the Potts model

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(Dated: February 2, 2008)

By relating the ground state of Temperley-Lieb hamiltonians to partition functions of 2D statistical mechanics systems on a half plane, and using a boundary Coulomb gas formalism, we obtain in closed form the valence bond entanglement entropy as well as the valence bond probability distribution in these ground states. We find in particular that for the XXX spin chain, the number  $N_c$  of valence bonds connecting a subsystem of size  $L$  to the outside goes, in the thermodynamic limit, as  $\langle N_c \rangle(\Omega) = \frac{4}{\pi^2} \ln L$ , disproving a recent conjecture that this should be related with the von Neumann entropy, and thus equal to  $\frac{1}{3 \ln 2} \ln L$ . Our results generalize to the  $Q$ -state Potts model.

PACS numbers: 03.67.-a 05.50+q

**Introduction.** Entanglement is a central concept in quantum information processing, as well as in the study of quantum phase transitions. One of the widely used entanglement measures is the von Neumann entanglement entropy  $S_{\text{vN}}$ , which quantifies entanglement of a pure quantum state in a bipartite system. To define  $S_{\text{vN}}$  precisely, let  $\rho = |\Psi\rangle\langle\Psi|$  be the density matrix of the system, where  $|\Psi\rangle$  is a pure quantum state. Given a complete set  $X$  of commuting observables, let  $X = A \cup B$  be a bipartition thereof. Then  $S_{\text{vN}}$  is defined as

$$S_{\text{vN}}(A) = -\text{Tr}_A \rho_A \ln \rho_A \quad (1)$$

where  $\rho_A = \text{Tr}_B \rho$  is the reduced density matrix with respect to  $A$ . One readily establishes that  $S_{\text{vN}}(A) = S_{\text{vN}}(B)$ . In most applications, the subset  $A$  corresponds to a commuting set of observables characterizing only a part of the whole system, and so one may think of  $A$  denoting simply that subsystem.

Critical ground states in 1D are known to have entanglement entropy that diverges logarithmically in the subsystem size with a universal coefficient proportional to the central charge  $c$  of the associated conformal field theory. Let  $L = |A|$  be the size of the subsystem, and  $N$  the size of the whole system, both measured in units of the lattice spacing, with  $1 \ll L \ll N$  (as we shall invariably assume in what follows). Then [1, 2]

$$S_{\text{vN}}(A) \stackrel{\text{a}}{=} (c/3) \ln L. \quad (2)$$

where by  $\stackrel{\text{a}}{=}$  we denote asymptotic behaviour. Away from the critical point, the entanglement entropy saturates to a finite value, which is related to the correlation length.

The von Neumann entanglement entropy is not an easy quantity to calculate, analytically or numerically; nor is it easy to grasp intuitively. The plethora of algebraic and geometric reformulations of quantum hamiltonians in one and higher dimensions [3, 4] suggests that there should be a more convenient, geometric way to define an

entanglement entropy. In the case of systems admitting infinite randomness fixed points, in one [5, 6, 7] as well as in higher [8, 9] dimensions, the ground state  $|\Omega\rangle$  can be represented as a single valence bond state, and  $S_{\text{vN}}$  coincides with the number of singlets that cross the boundary of  $A$  times the logarithm of the number of states per site.

In an interesting recent paper [10] (see also [11] for a related, independent work) it was suggested that, even when  $|\Omega\rangle$  is not a single valence bond state but a superposition of such states, the average number of singlets  $N_c(\Omega)$  crossing the boundary of the subsystem (multiplied e.g. by  $\ln 2$  for spins  $1/2$ ) could still be used as a measure of the entanglement entropy with all the required qualitative properties. Moreover, it was observed numerically in [10] that, up to statistical errors, this valence bond entanglement entropy  $S_{\text{vB}}$  had the same asymptotic behavior as  $S_{\text{vN}}$  for the XXX quantum spin chain, namely (2) with  $c = 1$ . In other words, the observation of [10] was that

$$\langle N_c \rangle(\Omega) \stackrel{\text{a}}{\approx} \frac{1}{3 \log 2} \ln L \simeq 0.481 \ln L. \quad (3)$$

Apart from this, the valence bond basis has been actively studied recently, in particular from rigorous [12, 13] and probabilistic [14] points of view.

Studying entanglement entropy from a geometrical point of view seems particularly appealing in view of the quantum dimer model of Rokhsar and Kivelson [15] and its many recent generalizations. Indeed, Henley [16] has shown that for *any* classical statistical mechanics model equipped with a discrete state space and a dynamics satisfying detailed balance, there is a corresponding quantum Hamiltonian whose ground state  $|\Omega\rangle$  is precisely the classical partition function. Of particular interest are then statistical mechanics models in which the microscopic degrees of freedom directly *define* the valence bonds. This is the case for a certain class of lattice models of loops, to be studied below.

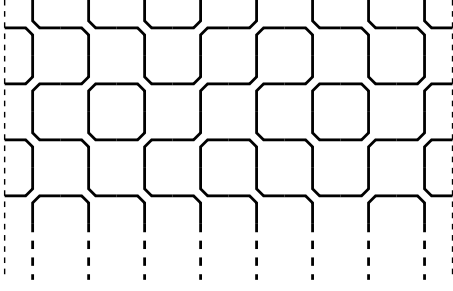


FIG. 1: Loop representation of the periodic TL algebra (with  $N = 8$ ) on the infinite half cylinder  $C_-$ . The basis state corresponding to the upper rim is  $\bullet(())\bullet$ .

We show in this Letter that the probability distribution of the number of singlets crossing the boundary can be exactly determined for the XXX spin chain as well as for the related  $Q$ -state Potts model hamiltonians. We find that (3) is not quite correct: the exact leading asymptotic behaviour is in fact  $\langle N_c \rangle(\Omega) \stackrel{a}{=} \frac{4}{\pi^2} \ln L \simeq 0.405 \ln L$ . All other cumulants have similar closed form expressions.

**Entanglement and the TL algebra.** The 2D classical  $Q$ -state Potts model can be defined for  $Q$  non integer through an algebraic reformulation where  $Q$  enters only as a parameter. For this, recall that the transfer matrix in the anisotropic limit gives rise to the hamiltonian [22]

$$H = - \sum_{i=1}^{N-1} e_i \quad (4)$$

Here the  $e_i$  are elements of an associative unital algebra called the Temperley-Lieb (TL) algebra, defined by

$$\begin{aligned} e_i^2 &= \sqrt{Q} e_i \\ [e_i, e_j] &= 0 \text{ for } |i - j| \geq 2 \\ e_i e_{i+1} e_i &= e_i \end{aligned} \quad (5)$$

The ground state of  $H$  depends on the representation of the algebra. For our purpose, it is natural to use the loop model representation, where the generators act on the following non-orthogonal but linearly independent basis states. Each basis state corresponds to a pattern of  $N$  parentheses and dots, such as  $()\bullet(())\bullet$ . The parentheses must obey the typographical rules for nesting, and the dots must not be inside any of the parentheses. These rules imply that the  $()$  pairs consist of one even and one odd site, and that dots are alternately on even and odd sites. We start by convention with an odd site on the left. Note that we have used an open chain for convenience, but that a periodic chain can be considered as well. This requires the introduction of an additional generator  $e_N$  coupling the  $N^{\text{th}}$  and first site, and in the graphical representation, parentheses can now be paired cyclically so  $)\bullet(())\bullet($  is now a valid pattern. This is shown in Fig. 1.

One can interpret these states in terms of spin  $1/2$  by associating with each pair of nearest parentheses  $()$  a

$U_q sl(2)$  singlet ( $\sqrt{Q} = q + q^{-1}$ ) so a valence bond can be drawn between the two corresponding sites. (Note that the generator  $e_i$  is nothing but the operator that projects sites  $i$  and  $i + 1$  onto the singlet.) For the dots, the state must be chosen such that the application of the projection operator onto the  $U_q sl(2)$  singlet for any two dots that are adjacent (when parentheses are ignored) annihilates the state. Thus those sites are “non-contractible”. With these definitions, it is clear that the TL algebra does not mix states with different numbers of non-contractible sites. For  $Q$  generic, the set of basis states with fixed number  $2j$  of such sites provides an irreducible representation of TL, of well-known dimension

$$d_j = \binom{N}{N/2 + j} - \binom{N}{N/2 + j + 1} \quad (6)$$

where  $N/2 + j$  must be an integer. This dimension coincides with the number of representations of spin  $j$  appearing in the decomposition of the product of  $N$  spins  $1/2$ . This is no accident: it is well-known [17] that the uncrossed diagrams are linearly independent and form a basis of the spin  $j$  sector in the  $sl(2)$  case; the results extends trivially to the  $U_q sl(2)$  case with  $q$  generic.

When  $\sqrt{Q} \geq 0$  the ground state is found in the sector with  $j = 0$  for  $N$  even (and  $j = 1/2$  for  $N$  odd). Note that the valence-bond basis is not orthonormal. The simplest way to proceed is thus not to calculate matrix elements of the hamiltonian  $H$  in this basis  $\langle w_i | H | w_j \rangle$  but rather to define a non-symmetric matrix  $h_{ij}$  by expressing the action of  $H$  on any state as a linear combination of states

$$H | w_i \rangle = \sum_j h_{ij} | w_j \rangle \quad (7)$$

The matrix  $h_{ij}$  is unique due to the linear independence of the states. The eigenvalues and right eigenvectors of  $h$  give those of  $H$ .

Since all entries  $h_{ij}$  are (strictly) positive, the Perron-Frobenius theorem implies that the ground state  $|\Omega\rangle$  expands on the basis words with positive coefficients [23]

$$|\Omega\rangle = \sum_w \lambda_w |w\rangle, \quad \lambda_w > 0 \quad (8)$$

We define the number of valence bonds  $N_c$  connecting the subsystem to the outside as the number of unpaired parentheses in the subsystem. We are here interested in its mean value

$$\langle N_c \rangle(\Omega) = \frac{\sum_w \lambda_w N_c(w)}{\sum_w \lambda_w} \quad (9)$$

and more generally in the probability distribution

$$p(N_c) = \frac{\sum_{w: N_c(w)=N_c} \lambda_w}{\sum_w \lambda_w} \quad (10)$$

Below we establish the leading asymptotic behaviour of  $\langle N_c \rangle$  (and the higher cumulants) in the scaling limit  $1 \ll$

$L \ll N$ . Note that the TL formulation shows relationship between the Potts hamiltonian when  $\sqrt{Q} = 2 \cos \frac{\pi}{k+2}$ , with  $k$  integer, and the interacting anyons (coming in  $k+1$  species) hamiltonian in [18]. The valence bond entanglement entropy can be defined for these models as well, and, in the sector of vanishing topological charge, coincides with the one we are studying.

**Mapping onto a boundary problem.** The wave function in the ground state of a certain hamiltonian with periodic (free) boundary conditions [24] can be obtained as the path integral of the equivalent Euclidian theory on a infinite half cylinder (annulus), denoted  $C_-$  (or  $A_-$ ). To translate this in statistical mechanics terms, note that if we consider the square lattice with axial (diagonal) direction of propagation [cf. Fig. 1], the hamiltonian belongs to a family of commuting transfer matrices describing the  $Q$ -state Potts model with various degrees of anisotropy. The ground state of all these transfer matrices is given by  $|\Omega\rangle$ . Let us chose for instance the particular case where the Potts model is isotropic, with coupling constant  $e^K = 1 + \sqrt{Q}$ . Now the ground state  $|\Omega\rangle$  can be obtained by applying a large number of times the transfer matrix on an arbitrary initial state (corresponding to boundary conditions at the far end of  $C_-$  or  $A_-$ ). Clearly, by the mere definition of the transfer matrix, this means that the coefficients of the ground state  $|\Omega\rangle$  on the words  $|w\rangle$  are (up to a common proportionality factor) equal to the partition function of the 2D statistical system on  $C_-$  or  $A_-$  with boundary conditions specified by  $|w\rangle$ .

We must now study such partition functions. We move immediately to the limit  $N \rightarrow \infty$ . We then have a system in the half plane, which, in the geometrical description, corresponds to a gas of loops with fugacity  $\sqrt{Q}$  in the bulk, with half loops ending up with open extremities on the boundary. To go to the continuum limit it is convenient to transform this loop model into a solid-on-solid model [19]. For this parametrize  $\sqrt{Q} = 2 \cos \pi e_0$  with  $0 \leq e_0 < 1$  [25] Give to all the loops an orientation, and introduce complex weights  $\exp(\pm \frac{i\pi e_0}{4})$  for the left and right turns. Since on the square lattice the number of left ( $n_L$ ) minus the number of right ( $n_R$ ) turns equals  $\pm 4$ , this gives closed loops the correct weight  $\sqrt{Q}$ . Meanwhile, loops ending on the boundary will get, with this construction, the weight  $\sqrt{Q}_b = 2 \cos \frac{\pi e_0}{2}$  since for them  $n_L - n_R = \pm 2$  [20]. Although no such boundary weight appeared in the initial lattice model and partition function, we note that for the fully packed loop model we are interested in it does not matter: the number of open loops touching the boundary is just  $N/2 - j$ , a constant.

Introducing this boundary loop weight allows complete mapping to the SOS model (or free six-vertex model). Now it is known that in the continuum limit, the dynamics of the SOS height variables turns into the one of a free bosonic field [19]. In a renormalization scheme where loops carry a constant height step  $\Delta\Phi = \pm\pi$ , the propagator of the field evaluated at two points  $x, x'$  on

the boundary reads, in the infinite size limit [20]

$$\langle \Phi(x) \Phi(x') \rangle_N = -\frac{1}{g} \ln |x - x'|^2 \quad (11)$$

where  $g = 1 - e_0$ . Here the subscript N indicates Neumann boundary conditions, corresponding to the presence of loop extremities on the boundary.

Let us now single out a segment of length  $L$  on this boundary and attempt to count the number of loops connecting this segment to the rest of the boundary. To do this we insert a pair of vertex operators, one at each a extremity of the segment,  $V = \exp[i(\pm e_1 + e_0/2)\Phi]$ . These operators do not affect the loops encircling the whole interval  $L$  since they modify the weight of such loops from  $e^{\pm i\pi e_0/2}$  to  $e^{\pm i\pi e_0/2} e^{\mp i\pi e_0} = e^{\mp i\pi e_0/2}$ , thus giving the same sum  $\sqrt{Q}_b$ . But for loops connecting the inside to the outside, the weight is now  $w = 2 \cos \pi e_1$ . The boundary dimension of the fields  $V$  is, using the propagator

$$h = \frac{4e_1^2 - e_0^2}{4g} \quad (12)$$

so their two-point function decays as  $L^{-2h}$ . We can then find the average number of loops separating two given points by taking appropriate derivatives, and setting  $e_1 = e_0/2$  in the end. This leads to our main result

$$\langle N_c \rangle(\Omega) \triangleq \frac{e_0}{\pi(1 - e_0)} \frac{2 \cos(\pi e_0/2)}{\sin(\pi e_0/2)} \ln L \quad (13)$$

For the XXX chain ( $e_0 = 0$ ) this reads  $\langle N_c \rangle \triangleq \frac{4}{\pi^2} \ln L \approx 0.405 \ln L$ , while for bond percolation ( $Q = 1$  or  $e_0 = 1/3$ ) we have  $\langle N_c \rangle \triangleq \frac{\sqrt{3}}{\pi} \ln L \approx 0.551 \ln L$ . The slope becomes 1 exactly as  $e_0 \rightarrow 1$ , or  $\sqrt{Q} \rightarrow -2$ . We note that the result for the XXX case is close but definitely different from the one proposed in [10].

It is amusing to observe that one can exactly interpret the valence bond as singlet contractions for an ordinary supergroup in the case  $Q = 1$ , by taking a lattice model where the fundamental three-dimensional representation of  $SU(2/1)$  and its conjugate alternate. The hamiltonian is again (4), but this time the  $e_i$  are projectors onto the singlet in  $3 \otimes 3$ . The effective central charge for the this spin chain is  $c_{\text{eff}} = 1 + \frac{9}{\pi^2} [\text{arccosh}(3/2)]^2 \simeq 1.845$ , and extending the argument suggested in [10] for the XXX case gives a slope of  $\frac{c_{\text{eff}}}{3 \ln 3} \simeq 0.559$ , even closer to the exact result (13).

Of course, by taking higher derivatives of the two-point function of the vertex operators one can access the higher moments of (10). In fact, the two-point function itself is nothing but the characteristic function of  $p(N_c)$ , although carrying out the Fourier transform in general is somewhat cumbersome. We will content ourselves here by giving the first few cumulants  $\mathcal{C}_k = (c_k/\pi^k) \ln L$ , with, in the XXX case (top) and the  $Q = 1$  case (bottom):

$$c_1 = \begin{cases} 4 \\ \sqrt{3}\pi \end{cases} \quad c_2 = \begin{cases} 8/3 \\ 2(2\pi\sqrt{3} - 9) \end{cases} \quad c_3 = \begin{cases} 16/15 \\ 8(5\pi\sqrt{3} - 27) \end{cases} \quad (14)$$

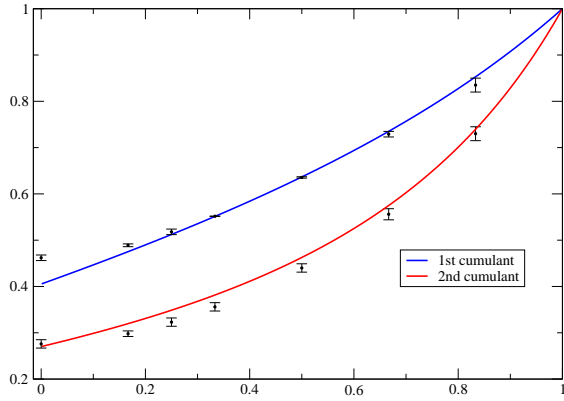


FIG. 2: Comparison between exact and numerically determined values of the slopes  $c_1$  and  $c_2$ , shown as functions of the parameter  $e_0$ .

together with the observation that, as  $\sqrt{Q} \rightarrow -2$ , the probability distribution becomes Poissonian:

$$\lim_{\sqrt{Q} \rightarrow -2} P(N_c) = e^{-\ln L} \frac{(\ln L)^{N_c}}{N_c!} \quad (15)$$

**Numerical calculations.** We have computed the distribution (10) numerically by exactly diagonalizing the transfer matrix, for periodic chains of size up to  $N_{\max} = 32$ . The cumulants  $\mathcal{C}_k \propto \ln L$  of  $p(N_c)$  obey a very simple finite size scaling (FSS) form, where  $\ln L$  has to be replaced by  $\frac{N}{\pi} \ln \sin \frac{L\pi}{N}$ ; this follows from standard formulas for two-point functions of our vertex operators  $V$ . Precise values of the slopes  $c_k$  can then be extracted from a careful analysis of the residual FSS effects. As shown in Fig. 2 they agree well with our analytical results, except for  $Q \rightarrow 4$ , where we expect logarithmic FSS corrections.

For  $Q = 1$ , the combinatorial nature of  $|\Omega\rangle$  implies that all  $\lambda_w$  in (8) are *integers*. This allows to obtain  $p(N_c)$  *exactly* for finite  $L$  and  $N \leq N_{\max}$ . Using this, we can in some cases conjecture  $p(N_c)$  for any value of  $N$  [21]. In particular we have established that

$$\langle N_c \rangle = (N^2 - L^2) p_k(N^2) \prod_{n=0}^{N/2-1} (N^2 - (2n+1)^2)^{n-N/2} \quad (16)$$

where  $p_k$  is a polynomial of degree  $k = \frac{1}{8}(N+4)(N-2)$  in  $N^2$ . This exact FSS form allows to obtain for the slope  $c_1 = 0.5517 \pm 0.0003$ , in very precise agreement with the value 0.551329 from (13).

**Conclusions.** As already argued in [10],  $S_{VB}$  is a measure of entanglement which seems as good qualitatively as  $S_{VN}$ , and easier to obtain numerically. We have shown in this Letter that it is also possible to tackle it analytically in the 1D case. The results are less easily expressed than for  $S_{VN}$  (which is proportional to  $c$ ). On the other hand, they fit considerably more naturally within the transfer matrix and Coulomb gas formalism. It remains to

be seen what happens for other models, and whether in particular a c-theorem of sorts is obeyed for  $S_{VB}$ .

**Acknowledgments.** We thank F. Alet for helpful exchanges, and for pointing out Ref. [18]. This work was supported by the European Community Network ENRAGE (grant MRTN-CT-2004-005616) and by the Agence Nationale de la Recherche (grant ANR-06-BLAN-0124-03).

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  - [22] The scale of (4) affects the sound velocity and is important when studying the scaling of gaps. But it does not matter when dealing with entanglement issues.
  - [23] Note that the scalar product of a state  $|w\rangle$  with itself is equal to  $\sqrt{Q}^{N/2-j}$  for all  $w$ , so there is no need to consider “normalized” basis words.
  - [24] The boundary conditions at large  $N$  are not expected to affect the leading behaviour of  $S_{VB}$ .
  - [25] When  $\sqrt{Q} < 0$  (i.e.  $\frac{1}{2} < e_0 < 1$ ) the true ground state has spin  $j > 0$ . Nevertheless, we continue to let  $|\Omega\rangle$  denote the  $j = 0$  ground state. Numerical studies then indicate that (8) holds even for  $\sqrt{Q} < 0$ , if  $N$  is large enough.